Noname manuscript No.
(will be inserted by the editor)

Electronic Supplementary Material for "Robust Accurate Identification and Biomass Estimates of Multiple Microorganisms via Tandem Mass Spectrometry"

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Received: date / Accepted: date

Supplementary Figures

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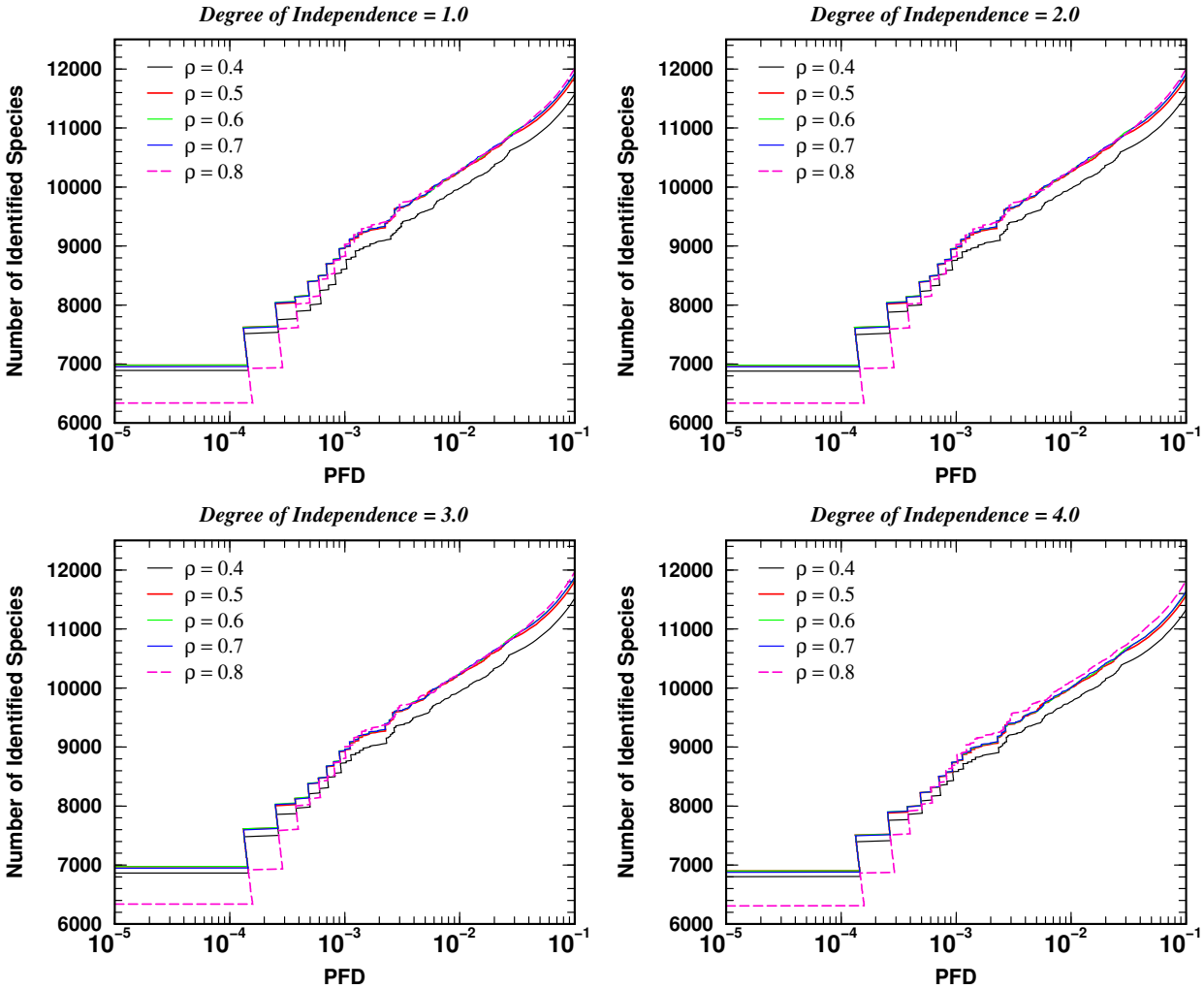

Fig. S1: Using the MS/MS spectra of BMD-A-1 as queries, we plot the retrieval curves (the number of species identified versus PFD) using various cutoffs for both degree of independence (specified on top of each panel) and resemblance coefficient (indicated by ρ's in the legend).

Table S1: List of MS/MS data files (DF's) downloaded from the ProteomeXchange (http://www.proteomexchange.org/) and from PeptideAtlas (http://www.peptideatlas.org/)

DF	Data File Name	Sample ID
Pseudomonas aeruginosa PA01		
1	QE_150611_152.raw	PXD004321
2	QE_150611_155.raw	PXD004321
3	QE_150611_158.raw	PXD004321
Staphylococcus aureus NTCTC 8325		
4	QE_150611_128.raw	PXD004321
5	QE_150611_131.raw	PXD004321
6	QE_150611_137.raw	PXD004321
Streptococcus pneumoniae CCUG 28588T		
7	QE_150508_32.raw	PXD004321
8	QE_150508_35.raw	PXD004321
9	QE_150508_38.raw	PXD004321
Escherichia coli K12		
10	QE_150611_140.raw	PXD004321
11	QE_150611_143.raw	PXD004321
12	QE_150611_146.raw	PXD004321
Moraxella catarrhalis CCUG 353T		
13	QE_160603_81.raw	PXD004321
14	QE_160603_84.raw	PXD004321
15	QE_160603_87.raw	PXD004321
Haemophilus influenzae CCUG 23945T		
16	QE_160627_44.raw	PXD004321
17	QE_160627_50.raw	PXD004321
18	QE_160627_52.raw	PXD004321
Mixture of 4 organisms [**?**]		
19	QE_150611_161.raw	PXD004321
20	QE_150611_164.raw	PXD004321
21	QE_150611_169.raw	PXD004321
22	QE_160819_05.raw	PXD004321
23	QE_160819_08.raw	PXD004321
24	QE_160819_11.raw	PXD004321
25	QE_160819_14.raw	PXD004321
26	QE_160819_17.raw	PXD004321
27	QE_160819_20.raw	PXD004321
28	QE_160819_44.raw	PXD004321
29	QE_160819_47.raw	PXD004321
30	QE_160819_50.raw	PXD004321
31	QE_160819_32.raw	PXD004321
32	QE_160819_35.raw	PXD004321
33	QE_160819_38.raw	PXD004321
34	QE_160819_23.raw	PXD004321
35	QE_160819_26.raw	PXD004321
36	QE_160819_29.raw	PXD004321
Mixture of 9 organisms [**?**]		
37	9MM_Run_1.raw	PASS00355
38	9MM_Run_2.raw	PASS00355
39	9MM_FASP.raw	PASS00355
40	9MM_PPID.raw	PASS00355
Mixture of 32 organisms [**?**]		
41	Run1_C1_2000ng.raw	PXD006118

Table S1: List of MS/MS data files (DF's) downloaded from the ProteomeXchange (http://www.proteomexchange.org/) and from PeptideAtlas (http://www.peptideatlas.org/)

42	Run1_C2_2000ng.raw	PXD006118
43	Run1_C3_1952ng.raw	PXD006118
44	Run1_C4_832ng.raw	PXD006118
45	Run1_P2_2000ng.raw	PXD006118
46	Run1_P3_2000ng.raw	PXD006118
47	Run1_P4_2000ng.raw	PXD006118
48	Run1_P1_96ng.raw	PXD006118
49	Run1_U1_2000ng.raw	PXD006118
50	Run1_U2_2000ng.raw	PXD006118
51	Run1_U3_2000ng.raw	PXD006118
52	Run1_U4_2000ng.raw	PXD006118
53	Run2_C1_2000ng.raw	PXD006118
54	Run2_C2_2000ng.raw	PXD006118
55	Run2_C3_2000ng.raw	PXD006118
56	Run2_C4_2000ng.raw	PXD006118
57	Run2_P2_2000ng.raw	PXD006118
58	Run2_P3_2000ng.raw	PXD006118
59	Run2_P4_2000ng.raw	PXD006118
60	Run2_P1_2000ng.raw	PXD006118
61	Run2_U1_2000ng.raw	PXD006118
62	Run2_U2_2000ng.raw	PXD006118
63	Run2_U3_2000ng.raw	PXD006118
64	Run2_U4_2000ng.raw	PXD006118
65	Run4_C1_2000ng.raw	PXD006118
66	Run4_C2_2000ng.raw	PXD006118
67	Run4_C3_2000ng.raw	PXD006118
68	Run4_C4_2000ng.raw	PXD006118
69	Run4_P1_2000ng.raw	PXD006118
70	Run4_P2_2000ng.raw	PXD006118
71	Run4_P3_2000ng.raw	PXD006118
72	Run4_P4_2000ng.raw	PXD006118
73	Run4_U1_4500ng.raw	PXD006118
74	Run4_U2_4600ng.raw	PXD006118
75	Run4_U3_4000ng.raw	PXD006118
76	Run4_U4_5300ng.raw	PXD006118
77	Run5_C2_2000ng.raw	PXD006118
78	Run5_C3_2000ng.raw	PXD006118
79	Run5_C4_2000ng.raw	PXD006118
80	Run5_P1_2000ng.raw	PXD006118
81	Run5_P2_2000ng.raw	PXD006118
82	Run5_P3_2000ng.raw	PXD006118
83	Run5_P4_2000ng.raw	PXD006118
84	Run5_U1_4500ng.raw	PXD006118
85	Run5_U2_4600ng.raw	PXD006118
86	Run5_U3_4000ng.raw	PXD006118
87	Run5_U4_5300ng.raw	PXD006118
MS/MS data of salive samples from 4 humans (2 females and 2 males) [**?**]		
88	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated1.raw	PXD003028
89	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated2.raw	PXD003028
90	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated3.raw	PXD003028
91	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated4.raw	PXD003028

Table S1: List of MS/MS data files (DF's) downloaded from the ProteomeXchange (http://www.proteomexchange.org/) and from PeptideAtlas (http://www.peptideatlas.org/)

92	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated5.raw	PXD003028
93	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated6.raw	PXD003028
94	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated7.raw	PXD003028
95	20150414_QEp1_LC7_NiGr_SA_Saliva_1_fractionated8.raw	PXD003028
96	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated1.raw	PXD003028
97	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated2.raw	PXD003028
98	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated3.raw	PXD003028
99	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated4.raw	PXD003028
100	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated5.raw	PXD003028
101	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated6.raw	PXD003028
102	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated7.raw	PXD003028
103	20150414_QEp1_LC7_NiGr_SA_Saliva_3_fractionated8.raw	PXD003028
104	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated1.raw	PXD003028
105	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated2.raw	PXD003028
106	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated3.raw	PXD003028
107	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated4.raw	PXD003028
108	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated5.raw	PXD003028
109	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated6.raw	PXD003028
110	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated7.raw	PXD003028
111	20150414_QEp1_LC7_NiGr_SA_Saliva_5_fractionated8.raw	PXD003028
112	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated1.raw	PXD003028
113	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated2.raw	PXD003028
114	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated3.raw	PXD003028
115	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated4.raw	PXD003028
116	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated5.raw	PXD003028
117	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated6.raw	PXD003028
118	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated7.raw	PXD003028
119	20150414_QEp1_LC7_NiGr_SA_Saliva_7_fractionated8.raw	PXD003028
MS/MS data of stool samples from 3 humans [?]		
DF	Data File Name	Sample ID
120	081915_H3_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
121	081915_H3_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
122	081915_H3_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
123	081915_H3_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
124	081915_H3_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
125	081915_H3_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
126	081915_H3_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
127	081915_H3_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
128	081915_H3_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
129	081915_H3_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
130	081915_H3_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
131	081915_H3_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
132	090115_H3_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
133	090115_H3_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
134	090115_H3_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
135	090115_H3_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
136	090115_H3_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
137	090115_H3_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
138	090115_H3_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
139	090115_H3_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
140	090115_H3_velos1_FTMS_MS2_hcd35_09.raw	PXD003907

Table S1: List of MS/MS data files (DF's) downloaded from the ProteomeXchange (http://www.proteomexchange.org/) and from PeptideAtlas (http://www.peptideatlas.org/)

141	090115_H3_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
142	090115_H3_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
143	090115_H3_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
144	090415_H3_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
145	090415_H3_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
146	090415_H3_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
147	090415_H3_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
148	090415_H3_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
149	090415_H3_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
150	090415_H3_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
151	090415_H3_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
152	090415_H3_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
153	090415_H3_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
154	090415_H3_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
155	090415_H3_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
156	082015_H4_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
157	082015_H4_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
158	082015_H4_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
159	082015_H4_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
160	082015_H4_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
161	082015_H4_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
162	082015_H4_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
163	082015_H4_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
164	082015_H4_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
165	082015_H4_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
166	082015_H4_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
167	082015_H4_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
168	090215_H4_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
169	090215_H4_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
170	090215_H4_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
171	090215_H4_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
172	090215_H4_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
173	090215_H4_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
174	090215_H4_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
175	090215_H4_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
176	090215_H4_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
177	090215_H4_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
178	090215_H4_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
179	090215_H4_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
180	090615_H4_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
181	090615_H4_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
182	090615_H4_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
183	090615_H4_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
184	090615_H4_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
185	090615_H4_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
186	090615_H4_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
187	090615_H4_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
188	090615_H4_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
189	090615_H4_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
190	090615_H4_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
191	090615_H4_velos1_FTMS_MS2_hcd35_12.raw	PXD003907

Table S1: List of MS/MS data files (DF's) downloaded from the ProteomeXchange (http://www.proteomexchange.org/) and from PeptideAtlas (http://www.peptideatlas.org/)

192	090315_H5_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
193	090315_H5_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
194	090315_H5_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
195	090315_H5_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
196	090315_H5_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
197	090315_H5_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
198	090315_H5_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
199	090315_H5_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
200	090315_H5_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
201	090315_H5_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
202	090315_H5_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
203	090315_H5_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
204	090715_H5_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
205	090715_H5_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
206	090715_H5_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
207	090715_H5_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
208	090715_H5_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
209	090715_H5_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
210	090715_H5_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
211	090715_H5_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
212	090715_H5_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
213	090715_H5_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
214	090715_H5_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
215	090715_H5_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
216	090915_H5_velos1_FTMS_MS2_hcd35_01.raw	PXD003907
217	090915_H5_velos1_FTMS_MS2_hcd35_02.raw	PXD003907
218	090915_H5_velos1_FTMS_MS2_hcd35_03.raw	PXD003907
219	090915_H5_velos1_FTMS_MS2_hcd35_04.raw	PXD003907
220	090915_H5_velos1_FTMS_MS2_hcd35_05.raw	PXD003907
221	090915_H5_velos1_FTMS_MS2_hcd35_06.raw	PXD003907
222	090915_H5_velos1_FTMS_MS2_hcd35_07.raw	PXD003907
223	090915_H5_velos1_FTMS_MS2_hcd35_08.raw	PXD003907
224	090915_H5_velos1_FTMS_MS2_hcd35_09.raw	PXD003907
225	090915_H5_velos1_FTMS_MS2_hcd35_10.raw	PXD003907
226	090915_H5_velos1_FTMS_MS2_hcd35_11.raw	PXD003907
227	090915_H5_velos1_FTMS_MS2_hcd35_12.raw	PXD003907
Escherichia coli K12		
228	Ecoli432_R1-rr_18Dec09_Falcon_09-09-14.mzXML	PXD001860
229	Ecoli432_R2_7Dec09_Falcon_09-09-15.mzXML	PXD001860
230	Ecoli432_R3_7Dec09_Falcon_09-09-16.mzXML	PXD001860
231	Ecoli432_R4_15Dec09_Falcon_09-09-16.mzXML	PXD001860
232	Ecoli433_R1_7Dec09_Falcon_09-09-14.mzXML	PXD001860
233	Ecoli433_R2_7Dec09_Falcon_09-09-15.mzXML	PXD001860
234	Ecoli433_R4_13Dec09_Falcon_09-09-16.mzXML	PXD001860
235	Ecoli434_R1_7Dec09_Falcon_09-09-14.mzXML	PXD001860
236	Ecoli434_R2_7Dec09_Falcon_09-09-15.mzXML	PXD001860
237	Ecoli434_R3_7Dec09_Falcon_09-09-16.mzXML	PXD001860
238	Ecoli434_R4_13Dec09_Falcon_09-09-16.mzXML	PXD001860
Mycobacterium tuberculosis H37Rv		
239	MtbH37Rv_03_run1_28Mar10_Draco_10-01-17.mzXML	PXD001860
240	MtbH37Rv_03_run2_28Mar10_Draco_10-01-15.mzXML	PXD001860

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241	MtbH37Rv_03_run3_28Mar10_Draco_10-01-15.mzXML	PXD001860
242	MtbH37Rv_04_run1_26Mar10_Draco_10-01-17.mzXML	PXD001860
243	MtbH37Rv_04_run2_28Mar10_Draco_10-01-15.mzXML	PXD001860
244	MtbH37Rv_04_run3_26Mar10_Draco_10-01-17.mzXML	PXD001860
245	MtbH37Rv_05_run1_26Mar10_Draco_10-01-17.mzXML	PXD001860
246	MtbH37Rv_05_run2_28Mar10_Draco_10-01-17.mzXML	PXD001860
247	MtbH37Rv_05_run3_28Mar10_Draco_10-01-15.mzXML	PXD001860
Salmonella typhimurium ATCC 14028		
248	SBEP_STM_286_2C_5Apr10_Falcon_10-01-23.mzXML	PXD001860
249	SBEP_STM_286_2D_15Apr10_Falcon_10-01-24.mzXML	PXD001860
250	SBEP_STM_287_2D_20Apr10_Falcon_10-01-24.mzXML	PXD001860
251	SBEP_STM_288_2C_5Apr10_Falcon_10-01-23.mzXML	PXD001860
252	SBEP_STM_288_2D_20Apr10_Falcon_10-01-24.mzXML	PXD001860
253	SBEP_STM_289_2C_1Apr10_Falcon_10-01-23.mzXML	PXD001860
254	SBEP_STM_289_2D_15Apr10_Falcon_10-01-24.mzXML	PXD001860
Yersinia pseudotuberculosis PB-1		
255	SBEP_YSTB_015_R1_28Sep10_Falcon_10-07-37.mzXML	PXD001860
256	SBEP_YSTB_015_R2_28Sep10_Falcon_10-07-39.mzXML	PXD001860
257	SBEP_YSTB_015_R3_10Oct10_Falcon_10-07-40.mzXML	PXD001860
258	SBEP_YSTB_016_R1_24Sep10_Falcon_10-07-37.mzXML	PXD001860
259	SBEP_YSTB_016_R2_24Sep10_Falcon_10-07-39.mzXML	PXD001860
260	SBEP_YSTB_016_R3_29Sep10_Falcon_10-07-40.mzXML	PXD001860
261	SBEP_YSTB_017_R1_28Sep10_Falcon_10-07-37.mzXML	PXD001860
262	SBEP_YSTB_017_R2_24Sep10_Falcon_10-07-39.mzXML	PXD001860
263	SBEP_YSTB_017_R3_29Sep10_Falcon_10-07-40.mzXML	PXD001860
Shewanella oneidensis MR-1		
264	QC_Shew_12_01_Run-07_21Jun12_Roc_12-04-08.mzXML	PXD001860
265	QC_Shew_12_01_Run-07_18Jun12_Roc_12-04-08.mzXML	PXD001860
266	QC_Shew_12_01_pt5_d_29Jun12_Jaguar_12-02-27.mzXML	PXD001860
267	QC_Shew_12_01_pt5_c_29Jun12_Jaguar_12-02-26.mzXML	PXD001860
268	QC_Shew_11-06_2p5_a_28May12_Polaroid_11-12-27.mzXML	PXD001860
269	QC_Shew_12_01_2p5_b_15Jun12_Polaroid_11-07-67.mzXML	PXD001860
270	QC_Shew_12_01_2p5_b_16Jun12_Polaroid_11-07-67.mzXML	PXD001860